Preprint
UCRL-JC-146976

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This article was submitted to XIV International Conference on Computational Methods in Water Resources, Amsterdam, The Netherlands, June, 2002

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

January 1, 2002

This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Applications of sensitivity analysis to uncertainty quantification in variably saturated flow

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In this paper, we present results demonstrating the effectiveness of a sensitivity analysis approach to uncertainty quantification of a variably saturated flow model. The basis for our method is a software system which simultaneously solves for solutions of large-scale nonlinear systems of equations and the sensitivity of the solutions to selected parameters. We present test cases showing the effects on the relative uncertainty of pressure due to heterogeneity in the absolute permeability and to differences in parameterizing the Van Genuchten curve soil parameters, α and n.

1. INTRODUCTION

Simulation of water resource management problems often requires the solution of large problems with many spatial zones. In addition, effective use of simulation solutions requires knowledge of the uncertainty introduced into the solution by variances in problem data. Current techniques for obtaining this information can require many runs of the simulation code and can be very time-consuming, especially for large-scale problems.

Sensitivity analysis techniques give a way to compute solution uncertainties by using information on the sensitivities of the solution to various parameters. These sensitivities are just the solution derivative with respect to the parameter in question, and equations for them can be derived by differentiating the original model equation. The resulting sensitivity equation is linear and can be solved in tandem with the model equations. Solution uncertainties can be developed from these sensitivities with a straightforward additional calculation.

Our model for variably saturated flow is the mixed form of Richards' equation [1],

$$\frac{\partial(s(p)\phi)}{\partial t} - \nabla \cdot \left(\frac{k k_r(p)}{\mu} \left(\nabla p - \rho g \nabla z \right) \right) = 0, \tag{1}$$

where $s(p)$ is water saturation, ρ is water density, ϕ is porosity of the medium, $k(x)$ is absolute permeability of the medium, $k_r(p)$ is relative permeability of water to air, μ is water viscosity, g is gravity and z is elevation.

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Discretization is done for time with an implicit backward differencing scheme and for space with a cell-centered finite difference scheme. One-point upstream weighting is used for the face values of relative permeability and harmonic averaging for the absolute permeability. Applying these discretization schemes leads to a set of coupled discrete nonlinear equations that must be solved at each time step.

This paper presents the application of a software system for the computation of solutions to large, nonlinear systems of equations as well as the computation of the sensitivities of the solution to various input parameters to a variably saturated flow model. The solution sensitivities are then used to compute a first order estimate of the solution uncertainties based on uncertainties in the Van Genuchten parameters.

2. UNCERTAINTY QUANTIFICATION and SENSITIVITIES

In this section we describe how sensitivities can be used to estimate uncertainties in the context of variably saturated flow problems. Relative permeability and saturation as functions of p can be modeled by Van Genuchten curves [2]. Often, the Van Genuchten curve soil parameters, α and n, are estimated using curve fits from data, thereby introducing error into the flow model. In addition, it is unclear as to how these parameters depend on the absolute permeability and whether this dependence impacts the problem solution. Thus, we model the α and n parameters as,

$$\alpha = a_1 ln|k| + a_2 \quad \text{and} \quad n = b_1 ln|k| + b_2 \tag{2}$$

where k is the absolute permeability of the medium which can exhibit heterogeneity, and the a_i and b_i are uncertain parameters. The main questions we want to answer are: *What is the uncertainty in the pressure caused by the uncertainties in the a_1, a_2, b_1, and b_2 parameters, and what is the sensitivity of pressure to changes in these parameters?*

We assume that we have a random sample of size N from the (a_1, a_2, b_1, b_2) population. A direct Monte Carlo sampling approach would be to solve (1) N times to find the mean and standard deviation of the resulting N pressure fields. Instead, we first let

$$\bar{a}_j \equiv \frac{1}{N}\sum_{i=1}^{N} a_{j,i} \quad \text{and} \quad \bar{b}_j \equiv \frac{1}{N}\sum_{i=1}^{N} b_{j,i} \tag{3}$$

be the corresponding sample means for $j = 1, 2$. We then solve (1) once using $a_j = \bar{a}_j$ and $b_j = \bar{b}_j$, denoting the nominal solution by $\tilde{p} \equiv p(\bar{a}_1, \bar{a}_2, \bar{b}_1, \bar{b}_2)$.

In the sensitivity analysis approach to uncertainty quantification, we use a first order Taylor series for $p(a_1, a_2, b_1, b_2)$ to approximate the dependence of p on the parameters a_1, a_2, b_1 and b_2. That is, we use

$$p(a_1, a_2, b_1, b_2) \approx \tilde{p} + \sum_{j=1}^{4} \left(\frac{\partial \tilde{p}}{\partial \gamma_j} \cdot (\gamma_j - \bar{\gamma}_j) \right), \tag{4}$$

where $\gamma_j \in [a_1, a_2, b_1, b_2]$. The derivatives $\partial p/\partial a_j$ and $\partial p/\partial b_j$ are called the *sensitivities* of p with respect to a_j and b_j. Equations for these derivatives can be obtained by differentiating (1) with respect to the a_j and b_j parameters.

Next, we want to use the above Taylor series approximation to obtain an estimate for the variance s_p^2 of the pressure about $\tilde{p}$ at each point in space. We define the vectors

$$\Delta\gamma_j \equiv \begin{pmatrix} \gamma_{1,j} - \bar{\gamma}_j \\ \vdots \\ \gamma_{N,j} - \bar{\gamma}_j \end{pmatrix}, \quad \text{and} \quad \Delta p \equiv \begin{pmatrix} p_1 - \tilde{p} \\ \vdots \\ p_N - \tilde{p} \end{pmatrix}.$$

Again using (4), we have

$$\Delta p \approx [\Delta a_1, \Delta a_2, \Delta b_1, \Delta b_2] \cdot \begin{pmatrix} \frac{\partial \tilde{p}}{\partial a_1} \\ \frac{\partial \tilde{p}}{\partial a_2} \\ \frac{\partial \tilde{p}}{\partial b_1} \\ \frac{\partial \tilde{p}}{\partial b_2} \end{pmatrix}.$$

Using these relationships, we can write

$$s_p^2 \approx \hat{s}_p^2 \equiv c^T V c, \quad \text{where} \quad c^T \equiv \left(\frac{\partial \tilde{p}}{\partial a_1}, \frac{\partial \tilde{p}}{\partial a_2}, \frac{\partial \tilde{p}}{\partial b_1}, \frac{\partial \tilde{p}}{\partial b_2} \right) \tag{5}$$

and

$$V \equiv \frac{1}{N-1} \cdot \begin{bmatrix} \Delta a_1^T \Delta a_1 & \Delta a_1^T \Delta a_2 & \Delta a_1^T \Delta b_1 & \Delta a_1^T \Delta b_2 \\ \Delta a_2^T \Delta a_1 & \Delta a_2^T \Delta a_2 & \Delta a_2^T \Delta b_1 & \Delta a_2^T \Delta b_2 \\ \Delta b_1^T \Delta a_1 & \Delta b_1^T \Delta a_2 & \Delta b_1^T \Delta b_1 & \Delta b_1^T \Delta b_2 \\ \Delta b_2^T \Delta a_1 & \Delta b_2^T \Delta a_2 & \Delta b_2^T \Delta b_1 & \Delta b_2^T \Delta b_2 \end{bmatrix}.$$

The matrix V is an approximation to the covariance matrix $C(a_1, a_2, b_1, b_2)$. The derivatives in the vector c are evaluated using calculated sensitivities.

Of course, the error $e = s_p^2 - \hat{s}_p^2$ depends upon how well the linear Taylor series approximations used above describe the true nonlinear behavior of the uncertainties. One could also extend this linear approach to a higher order method in the natural way. For example, a quadratic approach would require three additional solves for the extra sensitivities and would generally be more accurate, but it would most likely still be much less expensive than a full Monte Carlo sampling approach.

3. IMPLEMENTATION

We have implemented a three-dimensional variably saturated flow model based on Richards' equation in the ParFlow software package [3]. The Richards' equation model uses the KINSOL inexact Newton-Krylov [4] software package to solve the nonlinear systems at each time step [5]. Each nonlinear Newton iteration is solved with GMRES [6] preconditioned with Schaffer's semi-coarsening multigrid [7] method implemented in the *hypre* preconditioning library [8]. Previous work has shown that this solution method is very effective for variably saturated flow problems [9].

After discretization, the nonlinear equation for each finite difference point $x_{i,j,k}$ at each time step can be written in the form

$$F_{i,j,k}(p) = 0, \tag{6}$$

where F is the nonlinear function expressing the discrete form of (1), and p is the vector of pressures at the new time level at the finite difference points. Thus, at each time step, we have the coupled nonlinear system

$$F(p, a_1, a_2, b_1, b_2) = 0 \tag{7}$$

to solve for all the discrete pressure values. Note that the dependence on the uncertain parameters has explicitly been included in this system even though these parameters enter the model through the expressions for relative permeability and saturation.

Next, we define $S_j = \tilde{\gamma}_j \frac{\partial p}{\partial \gamma_j}$ for $\gamma_j \in [a_1, a_2, b_1, b_2]$ as the scaled sensitivity of pressure to the parameter γ_j. The $\tilde{\gamma}_j$ are nominal values used only for scaling. Differentiating (7) with respect to each of the parameters gives the equation,

$$\frac{\partial F}{\partial p} S_j + \tilde{\gamma}_j \frac{\partial F}{\partial \gamma_j} = 0. \tag{8}$$

This differentiation gives a linear equation for each of the 4 sensitivities we seek.

We calculate the solutions to these equations with the sensitivity version of KINSOL [10]. This software package solves the nonlinear system at a time step, then uses the solution to form (8) for each of the four parameters. First, $\frac{\partial F}{\partial \gamma_j}$ and the Jacobian of F given by $\frac{\partial F}{\partial p}$ are evaluated. SensKINSOL evaluates the derivatives of the F with respect to the parameters, γ_j, by taking finite differences of F as in

$$\frac{\partial F}{\partial a_1} \approx \frac{F(p, a_1 + \delta_{a_1}, a_2, b_1, b_2) - F(p, a_1 - \delta_{a_1}, a_2, b_1, b_2)}{2\delta_{a_1}}, \tag{9}$$

and similarly for the other derivatives of F. One could also use automatic differentiation techniques, and future releases of SensKINSOL will provide basic interfaces to the automatic differentiation software, ADIC [11]. SensKINSOL then solves these systems using the same linear solver and preconditioner as is used in the solution of the nonlinear iterations.

4. NUMERICAL RESULTS

To explore the sensitivity and uncertainty of pressures, we have constructed a test case with a large, deep vadose zone and a long-term infiltration study [12]. The alluvial site was modeled both as an anisotropic homogeneous system (case A) and as two isotropic heterogeneous systems (cases B and C). In case B Van Genuchten parameters are not correlated to saturated hydraulic conductivity, and in case C, α in (2) is correlated to saturated hydraulic conductivity but n is not. These cases are summarized in Table 1. The domain geometry was $150\mathrm{m} \times 150\mathrm{m} \times 250\mathrm{m}$ with a trench of $3\mathrm{m} \times 150\mathrm{m} \times 250\mathrm{m}$ infiltrating in the upper left of the domain with a rate of $5\mathrm{m}^3/\mathrm{d}$. A $25 \times 15 \times 50$ grid was used with cell spacings of $6\mathrm{m} \times 10\mathrm{m} \times 5\mathrm{m}$. For the homogeneous cases, the saturated hydraulic conductivity was set to $3.6\mathrm{m/d}$ in the x and y directions and $0.517\mathrm{m/d}$ in the z direction. For the two heterogeneous cases, the hydraulic conductivity was assumed to be isotropic and described by a correlated, Gaussian random field, generated numerically via the turning bands algorithm [13]. A geometric mean of $7.5\mathrm{m/d}$ with correlation lengths in the x, y, and z directions of $25\mathrm{m}, 12\mathrm{m}$, and $6\mathrm{m}$, respectively, and a variance of the log of hydraulic conductivity of 1.5 was used. For the heterogeneous cases, three realizations of permeability with different random seeds were simulated for comparison.

Table 1
This table gives the values of a_1, a_2, and b_2 used in the variations on our basic test case. The % standard deviation used for parameter c is denoted by σ_c. Note that b_1 and its standard deviation were taken as 0 for all cases.

Case	a_1	σ_{a_1}	a_2	σ_{a_2}	b_2	σ_{b_2}	k	Random Seed
A	0.0	0%	9.0	10%	1.5	1%	Hom.	N/A
B	0.0	0%	9.0	10%	1.5	1%	Het.	3
C	0.9927	10%	6.9998	10%	1.5	1%	Het.	3

Saturation fields are shown in Figure 1 at 260 days for the three cases. We see the effects of the trench infiltrating down into the vadose zone. Case C shows much more dependence on the heterogeneity in the permeability field than the other two. This increased dependence is due primarily to the dependence of α in (2) on k.

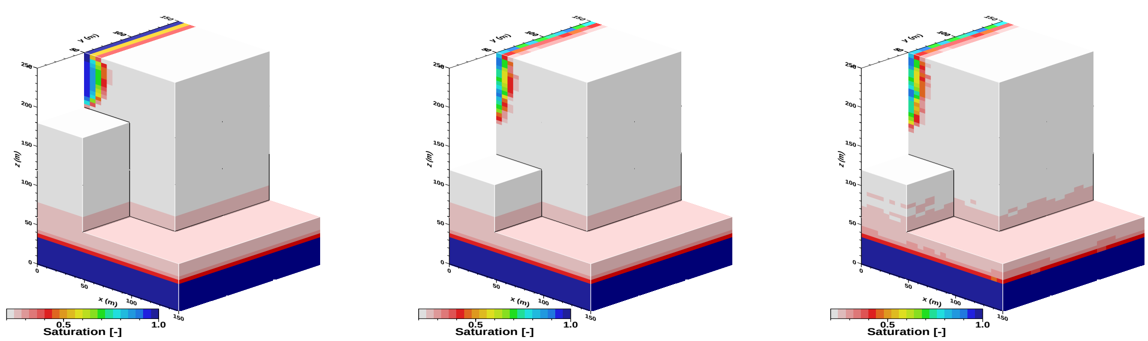

Figure 1. Saturation fields for the three cases at 260 days show varying impacts of heterogeneity. Case A (left) shows little impact, while cases B and C show increased impacts.

For cases A and B, sensitivities were computed for a_2 and b_2, and for case C, sensitivities were also computed for a_1. The sensitivities (unscaled) of pressure to a_1, a_2, and b_2 for case C are shown in Figure 2. We see that the sensitivity to a_1 is greater than to a_2 indicating that the heterogeneity is an important factor in the computed values of pressure. Also, the pressures are much more sensitive to b_2 than the other parameters. Cases A and B show the same relative sensitivity of the a_2 and b_2 parameters. This trend indicates that an accurate value of n is much more critical to this test case than an accurate value of α. We see this to be true in Table 2 where % uncertainties are shown for the three test cases at varying times. The final columns of this table give an estimate of the percent of the uncertainty contributed by a percent standard deviation given in Table 1 for each of the three parameters. Clearly b_2 with a 1% standard deviation contributes most to the uncertainty in the domain averaged pressure.

Table 2 also shows the % uncertainty of the domain averaged pressure for cases B and C with

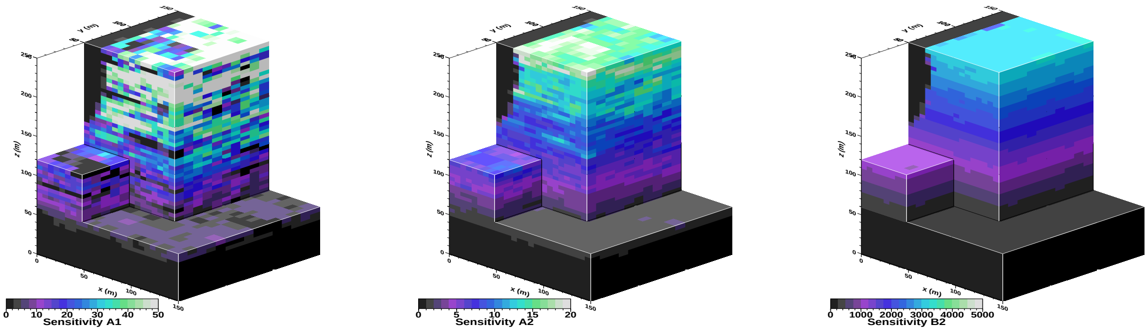

Figure 2. This figure shows unscaled sensitivities of pressure to changes in the a_1, a_2, and b_2 parameters. The figure indicates that n is a much more important parameter to this test case than α in the Van Genuchten curves as noted by the different scales of absolute sensitivity for the three parameters in this case.

different seeds to the geostatistical model. Although we show results for only three realizations of the permeability field, we see that each of these realizations produces a similar mean and standard deviation of uncertainty when averaged across the domain, though local minima and maxima of uncertainty are realization dependent. There is indication of a slight but consistent decrease over time in the variance due to b_2.

Figure 3 shows the total relative uncertainties for the three cases at 260 days. These uncertainties were computed using the standard deviations given in Table 1 and (4). We see that uncertainties are much lower in the more saturated areas in the water table and near the trench. In these areas, of course, the relative permeabilities and saturations are less dependent on the parameters in the Van Genuchten curves. In addition, we see less uncertainties overall in case C indicating that accounting for the heterogeneity in the Van Genuchten parameters may reduce overall uncertainty in the final pressure solutions.

5. CONCLUSIONS

Solutions and solution sensitivities for variably saturated flow problems can be solved for simultaneously. In the case of Van Genuchten curves for relative permeability and saturation, sensitivity analysis has shown that our test case solutions are much more sensitive to n than α and that incorporating heterogeneity in the formulation of α does not dramatically change estimates of uncertainty. In the future, the first order estimates of uncertainty computed here will be compared with a Monte Carlo simulation approach.

ACKNOWLEDGMENTS

The authors would like to thank Steven G. Smith for his valuable assistance with the ParFlow code package, Peter Brown for discussions on the computation and use of sensitivities, Steve

Table 2
Spatially averaged percent uncertainties of pressure for different heterogeneity cases, random seeds, and times. The standard deviation of the percent uncertainty is denoted by σ. The final three columns show the approximate percentage contributions to the variance from parameters a_1, a_2, and b_2.

Case	Seed	Day	% Unc.	σ	$\%\sigma^2{}_{a_1}$	$\%\sigma^2{}_{a_2}$	$\%\sigma^2{}_{b_2}$
A	N/A	20	2.1956e+01	2.8896e+00	0.0	20.7	79.3
A	N/A	60	2.1904e+01	2.8837e+00	0.0	21.0	79.0
A	N/A	260	2.1472e+01	3.4097e+00	0.0	22.0	78.0
B	3	20	2.1946e+01	2.9223e+00	0.0	20.7	79.3
B	3	60	2.1837e+01	3.0185e+00	0.0	21.0	79.0
B	3	260	2.1291e+01	3.6151e+00	0.0	22.3	77.7
B	33	20	2.1962e+01	2.8559e+00	0.0	20.7	79.3
B	33	60	2.1850e+01	2.9706e+00	0.0	21.0	79.0
B	333	20	2.1991e+01	2.7706e+00	0.0	20.7	79.3
B	333	60	2.1857e+01	3.0048e+00	0.0	20.9	79.1
C	3	20	2.1225e+01	2.9623e+00	1.0	13.9	85.0
C	3	60	2.1090e+01	3.1476e+00	1.1	14.1	84.8
C	3	260	2.0567e+01	3.7458e+00	1.1	15.0	83.9
C	33	20	2.1238e+01	2.9062e+00	1.0	14.1	84.9
C	33	60	2.1125e+01	3.0217e+00	1.0	14.3	84.7
C	333	20	2.1256e+01	2.9161e+00	1.0	14.0	84.9
C	333	60	2.1168e+01	2.9783e+00	1.1	14.2	84.7

Carle for the development and assistance with the “Chunk” visualization package, and Andy Tompson for information on the test problem.

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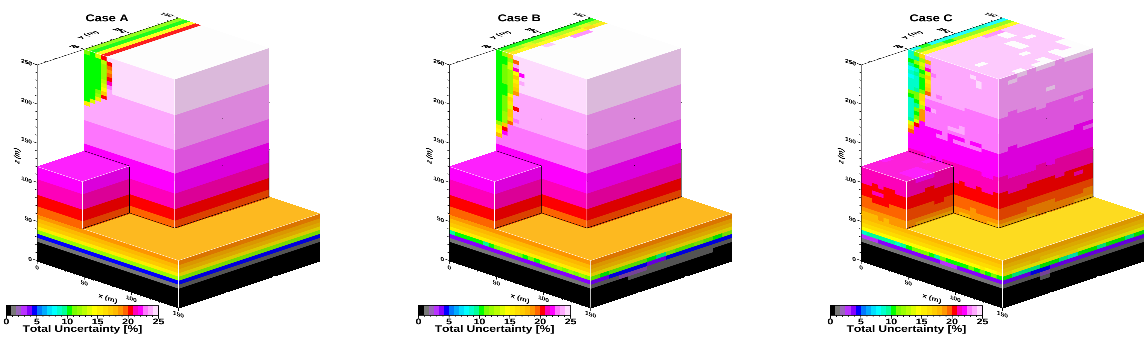

Figure 3. Percent uncertainties for the three cases show greater uncertainties away from saturated areas. Case A (left) has the highest uncertainty, and case C (right) has the least.

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